

# The overdoped regime in $La_{2-x}Sr_xCuO_4$

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Recent experimental data for the overdoped  $La_{2-x}Sr_xCuO_4$  have firmly established the properties which characterize the transition between the superconducting and the Fermi liquid metallic phases ( $\tilde{x} \simeq 0.25$ ). The thermodynamic response functions show a pronounced feature at this point, while the Fermi surface undergoes a dramatic change. By use of the Composite Operator Method for the two-dimensional Hubbard model, it is found that the presence of a van Hove singularity in the lower Hubbard band can explain these behaviors.

74.72.-h, 71.10.Fd, 71.10.-w

In the last few years the availability of single-crystal samples for overdoped  $La_{2-x}Sr_xCuO_4$  (LSCO) has permitted an experimental analysis [1] of the critical point which signs the transition between the superconducting and the Fermi liquid metallic phases ( $\tilde{x} \simeq 0.25$ ) [2,3].

At this value of dopant concentration some thermodynamic properties result to be greatly enhanced with a strongly pronounced peak. Indeed, this is the case for the entropy [4,3] and the uniform static spin magnetic susceptibility [3]. Further, at the same doping, the Hall coefficient reverses its sign [5] and an abrupt change in the shape of the Fermi surface occurs [1]. This kind of behavior could be seen as a clear indication of the crossing of a van Hove singularity through the chemical potential for that doping value ( $\tilde{x} \simeq 0.25$ ) or, ultimately, of the relevance of band dispersion driven processes in the overdoped region.

These experimental findings can be explained within an unique theoretical framework where the electronic state evolution at large hole doping is governed by a van Hove singularity. Beyond, this scenario is only sensitive to the location of the peak and not to the overall band structure.

By means of the Composite Operator Method, in the two-pole approximation [6], we have studied the two-dimensional Hubbard model and, in particular, the specific role played by the van Hove singularity in the lower Hubbard band.

The 2D Hubbard model is defined as follows:

$$H = \sum_{ij} t_{ij} c^\dagger(i) c(j) + U \sum_i n_\uparrow(i) n_\downarrow(i) - \mu \sum_i n(i) \quad (1)$$

where  $c(i)$  is the electron operator at the site  $i$ , in the spinor notation.  $t_{ij}$  denotes the transfer integral and describes hopping between nearest neighbor sites;  $U$  is the Hubbard interaction between two  $c$  electrons at the same site with  $n_\sigma(i)$  being the number operator per spin  $\sigma$ .  $\mu$  is the chemical potential and  $n(i)$  the total number operator.

As basic field for the causal thermal Green's function of the system we have chosen the Hubbard doublet. This

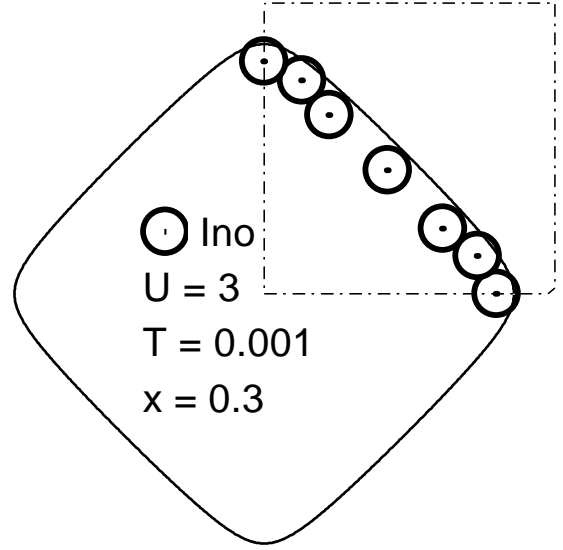


FIG. 1. Fermi surface for  $U = 3$ ,  $T = 0.001$  and  $x = 0.3$ . The experimental data  $\odot$  are taken from Ref. [1].

choice is dictated by the equations of motion of the basic electronic field  $c(i)$  and has the advantage to automatically preserve the first four spectral momenta [7]. In addition, it is known (quantum Monte Carlo and Lanczos data) that due to the on-site Coulomb interaction two sharp features develop in the band structure which correspond to the Hubbard subbands and describe interatomic excitations mainly restricted to subsets of the occupancy number [8]. The use of a non-standard basis gives us the possibility to implement a constraint on the solution with the content of the Pauli principle [6].

The analytical expressions for the entropy, the uniform static spin magnetic susceptibility and the Fermi surface have been already given in Refs. [9–11]. The entropy has been calculated by exploiting thermodynamic relations after the Maxwell's identities [9]; the spin magnetic susceptibility has been determined by use of the equations of motion [10]. The Fermi surface is given by the inter-

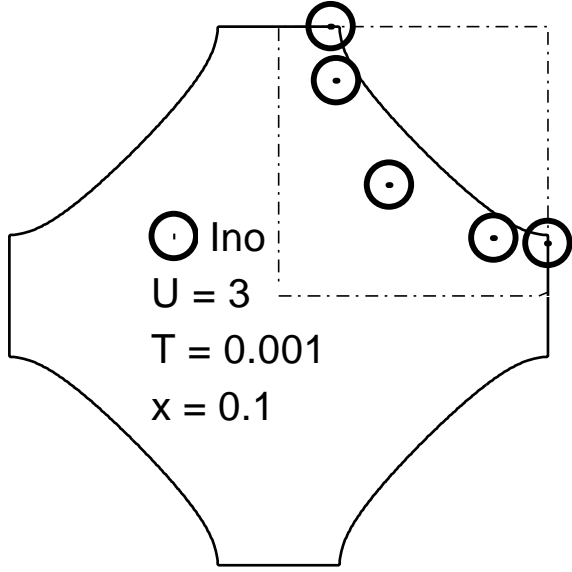


FIG. 2. Fermi surface for  $U = 3$ ,  $T = 0.001$  and  $x = 0.1$ . The experimental data  $\odot$  are taken from Ref. [1].

section between the lower Hubbard band and the energy level corresponding to the chemical potential [11].

The Fermi surface structure at  $x = 0.3$  for the *LSCO* has been only recently obtained by means of *ARPES* experiments [1]. The experimental data can be reproduced in the context of the two-dimensional one-band Hubbard model with  $U = 3$ , see Fig. 1. Both the shape and the volume of the Fermi surface qualitatively agree with experimental ones (errors of the order of 15%) showing that the nature of the metallic phase is of a conventional Fermi liquid state. In fact, it should be considered as experimentally robust that the destruction of the Fermi surface and the relative issue of a novel state of the matter arise only in the underdoped region [12].

The comparison with the experimental results [1] for  $x = 0.1$ , see Fig. 2, and  $x_c = 0.15$  shows that the Fermi surface changes its nature at a doping level between 0.15 and 0.3 in agreement with the Hall coefficient experiments [5]. The latter set this critical doping at the same value at which the superconductivity disappears [2] and all the thermodynamic properties related to the value of the density of states at the Fermi level present a pronounced maximum ( $\tilde{x} \simeq 0.25$ ) [4,3]. Our results for both the uniform static spin magnetic susceptibility and the entropy show these features at the same doping level ( $\tilde{x} \simeq 0.25$ ) and for the same values of the model parameters ( $U = 3$ ), see Fig. 3. A sharp maximum is well developed and reproduces the experimentally observed one [4,3]. In particular, a pronounced maximum in the uniform static spin magnetic susceptibility is a strong evidence for a pseudo-nesting effect when accompanied by evidences of an ordinary Fermi liquid phase.

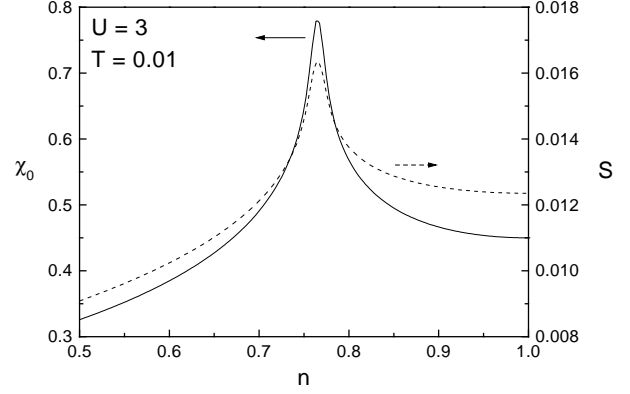


FIG. 3. The uniform static spin magnetic susceptibility  $\chi_0$  and the entropy  $S$  for  $U = 3$ ,  $T = 0.01$  as a function of the filling  $n$ . The left and right vertical scale refer to the intensity of  $\chi_0$  and  $S$ , respectively.

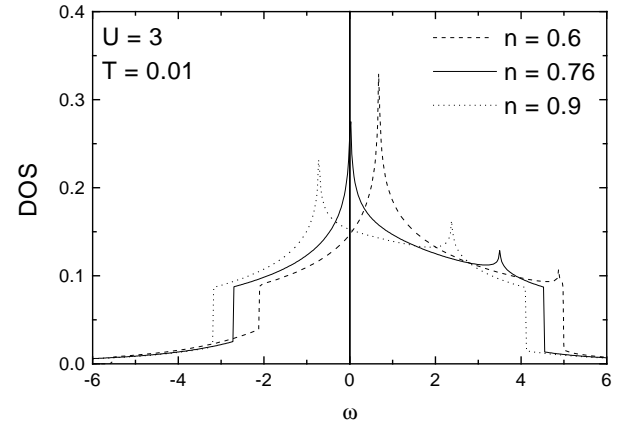


FIG. 4. Density of States for  $U = 3$ ,  $T = 0.01$  and different values of the filling  $n$ .

Now, analyzing the density of states for the same values of the model parameters, see Fig. 4, we can see that at the same doping level ( $\tilde{x} \simeq 0.25$ ) the lower Hubbard band van Hove singularity crosses the chemical potential. It is worth to note that it seems necessary to include second and third neighbor hopping to provide both the dispersion and the line shape of the *ARPES* data for the large variety of high- $T_c$  cuprates [13].

In conclusion, we have shown that the experimentally observed features in the overdoped region can be described by the relative position of the lower Hubbard band van Hove singularity. The latter crosses the Fermi level at some critical doping ( $\tilde{x} \simeq 0.25$ ) enhancing the density of states and changing the Fermi surface nature.

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